

# The spin - $\frac{1}{2}$ Heisenberg model on Kagome lattice as a quantum critical system

Tao Li

*Department of Physics, Renmin University of China, Beijing 100872, P.R.China*

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Through exact diagonalization study of the spin -  $\frac{1}{2}$  Heisenberg model on Kagome lattice with ring-exchange coupling  $J_r$ , we find the pure Heisenberg model with  $J_r = 0$  stands as a quantum critical point, as evidenced by avoided level crossing and divergence of the second derivative of the ground state energy with respect to  $J_r$  at  $J_r = 0$ . The pure Heisenberg model should thus be gapless in the thermodynamic limit, contrary to common beliefs. At the same time, the ring exchange coupling is found to drive the system into a state with more short ranged spin correlation and with a local spin correlation pattern equivalent to that of the antiferromagnetic Heisenberg model on triangular lattice (the peak of spin structure factor moves to the momentum  $\vec{q} = (\frac{4\pi}{3}, 0)$ ). The resemblance of state with the Marston-Zeng spin Pereils solid state (in terms of dimer-dimer correlation) is also much enhanced by the ring exchange coupling, although it is unclear if such correlation would solidify into static order in the thermodynamic limit.

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The spin liquid state represents a novel state of matter beyond the Landau-Ginzburg description and supports new kinds of order and excitation. It is generally believed that the geometrically frustrated quantum antiferromagnetic systems are ideal places to find spin liquid ground state[1]. The antiferromagnetic Heisenberg model on Kagome lattice, which is a typical frustrated system, is a especially promising target[2]. The geometric frustration of the Kagome system is so strong that the classical spin defined on such a lattice posses extensive ground state entropy. Understanding how quantum fluctuation would lift such huge degeneracy stands as a big challenge to both condensed matter theory and our imagination.

Much efforts, both in theory and experiment[3], has been devoted to the understanding of its exotic ground state and excitation properties. Earlier numerical studies on finite size systems have accumulated strong evidence for a spin disordered ground state with no symmetry breaking and a very short ranged spin correlation[4–15]. What makes the Kagome system even more extraordinary is the fact the spin gap is extremely small[9–13], although the spin correlation length is estimated to be only of the order of one lattice constant. At the same time, the singlet excitation channel is found to be abundant of low energy excitations below the spin gap[9, 10, 16–20], whose origin is still unclear[2, 18, 21–25]. All these characteristics are not what one expect for a typical spin liquid state with short range spin correlation and have puzzled people in the field for more than two decades.

It is now generally believed that a small but finite spin gap exists in the thermodynamic limit[9, 11–13, 17]. The same is also believed to be true for the excitation gap in the singlet channel[12, 13]. The ground state of the Heisenberg model on Kagome lattice is thus believed to be still consistent with our understanding for a nominal incompressible and featureless quantum liquid, although the excitation gap is very small for some unknown rea-

sons. However, since all these results are all derived from studies on finite size system and the low energy spectral weight of the system is very susceptible to local perturbations[18] as a result of the remarkable softness of the spin dynamics of the system[4], it is very susceptible that the observed excitation gap may simply be the artifact of the finite size effect or boundary effect. Slave Boson mean field analysis has predicted a critical state with Dirac type spinon dispersion as the ground state[28], which is shown later by Variational Monte Carlo calculation to be a good variational state in terms of energy[29]. However, many earlier numerical findings, especially the large amount of singlet excitation spectral weight below the spin gap (on finite size system), can not find a natural understanding in such a description.

Here we are especially interested in the low energy excitation in the singlet channel. Taking it literally, the aggregation of the large amount of spectral weight at such a low energy can be interpreted as a result of quasi-degeneracy of the ground state, which also implies the sensitivity of the ground state on small perturbations. A close analog of this situation can be found in a fractionally filled lowest Landau level, in which case the Coulomb repulsion will reorganize the system into an incompressible quantum liquid- the fractional quantum Hall state. It is very interesting to see if similar thing can happen in the Kagome system if we turn on some relevant perturbation.

Along this line of thinking, we suggest to study the spin -  $\frac{1}{2}$  Heisenberg model on Kagome lattice with ring exchange coupling. The model is given as follows

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_r \sum_{\text{hexagons}} (P + P^{-1}), \quad (1)$$

in which  $J_r$  denotes the ring exchange coupling constant on each hexagonal plaquette of the Kagome lattice (shown in Fig.1),  $P$  denotes the operator for cyclic permutation of the six electron on a hexagonal ring. It should be noted

that the ring exchange coupling on hexagonal plaquette represents the lowest order correction to the pure Heisenberg model in the large  $U$  expansion of the Hubbard model. For realistic systems,  $J_r$  should have a positive sign. It is the purpose of this paper to determine if such a correction would constitute a relevant perturbation on the physics of the pure Heisenberg system. Especially, we want to see if the ring exchange coupling would play a similar role as the Coulomb repulsion in fractionally filled lowest Landau level system and drive the system into an incompressible quantum liquid that match our general expectation for a spin liquid with short range spin correlation.

The effect of the ring exchange coupling has been studied extensively on frustrated quantum magnet. Earlier numerical study has found on triangular lattice that the ring exchange coupling may drive the system into a spin liquid state from the three sublattice magnetic ordered state[30]. However, the nature of the obtained spin liquid state is still under debate. Some author proposed a gapless spin liquid state with spinon Fermi surface based on mean field analysis[31] but others believe that some kind of spin gap exist[32].

To settle down the issue of the effect of the ring exchange coupling on the Kagome Heisenberg model, we have carried out exact diagonalization study on a Kagome cluster with 36 sites(shown in Fig.1). Such a finite cluster has the important property that it respects all the symmetry of the original Hamiltonian in the thermodynamic limit. Such symmetries are believed to be crucial to the understanding of delicate physics of the Kagome Heisenberg system. For example, numerical study shows that the low energy singlet dynamics of Kagome Heisenberg system, which stands as its characteristic exoticness, can be easily quenched by tiny amount of vacancy in the lattice[18]. The structure of the 36-site cluster is shown in Figure 1. The same cluster is first used in a exact diagonalization study of the pure Heisenberg model by Leung and Elser in 1993[7]. Here we have adopted the same numbering of sites and bonds as their choice for comparison of results.

In our study, we have concentrated on the fully symmetric subspace in which the ground state resides. This subspace, which belongs to the identity representation of the symmetry group, has 31527894 basis vectors. We have used both the Lanczos and the Arnoldi algorithm[26] to calculate the ground state properties and the lowest excitation in the fully symmetric subspace. Lanczos calculation of the lowest eigenvalue in general irreducible representations at high symmetry momentum is carried out also to make sure that ground state indeed resides in the fully symmetric subspace. To uncover the nature of the ground state found, we have calculated the spin-spin correlation and dimer-dimer correlation function on the cluster.

Although the physical ring exchange coupling should

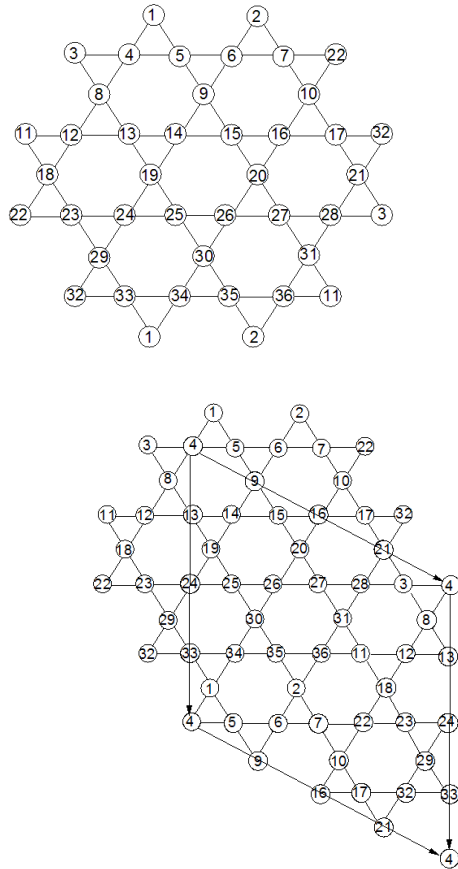


FIG. 1: The 36-site Kagome cluster on which our exact diagonalization study is performed. Our numbering of the lattice sites is the same as that used in Ref[7]. In the upper panel, the cluster is presented in such a way that the rotational symmetry of the cluster is explicit, while in the lower panel, it is presented in such a fashion that the boundary condition on the cluster is explicit.

be positive, we will treat  $J_r$  as a free controlling parameter that can take both positive and negative values. In Figure 2, we plot the ground state energy and the lowest excitation energy in the fully symmetric subspace as functions of  $J_r$ . The most striking thing in this figure is the fact that an avoided level crossing occurs exactly at the pure Heisenberg limit, namely at  $J_r = 0$ .

An avoided level crossing in the spectrum of a finite system is a signature of the quantum phase transition[27]. As the size of the lattice grows, the crossing will become progressively sharper and eventually lead to a non-analyticity in ground state energy in the infinite lattice limit. Thanks to the short ranged nature of the spin correlation in the ground state of the pure Heisenberg model, the 36-site cluster system already exhibits quite sharp level crossing. To make it clearer, we plot in Figure 2 also the difference of the crossing energies as a function

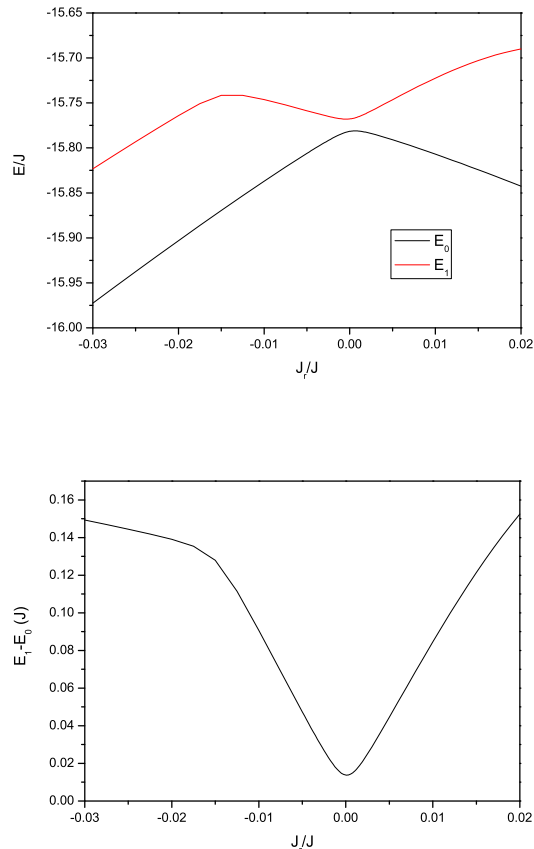


FIG. 2: Upper panel: The lowest two eigenvalues in the fully symmetric subspace as functions of the ring exchange coupling. Avoided level crossing is clearly seen around the pure Heisenberg limit at  $J_r = 0$ . Lower panel: the difference in the lowest two eigenvalues as a function of  $J_r$ .

of  $J_r$ .

Now we focus on the ground state properties. As the transition is driven by the ring exchange coupling, we plot the first and the second derivative of the ground state energy as a function of  $J_r$  in Fig. 4. According to the Hellmann-Feynman theorem, the first derivative is just the expectation value of the ring exchange coupling in the ground state. It is expected that such coupling should engage in a dramatic change acrossing the transition point at  $J_r = 0$ , as is clear in the figure. The second derivative shown in Fig. 4(b) exhibits the typical divergence during a quantum phase transition, although the calculation is done on a still relatively small lattice of 36 sites. The pure Heisenberg model on Kagome lattice is thus a quantum critical point. As a result, the gap in the spin channel and singlet channel should all vanish in the thermodynamic limit. This is contrary to the common beliefs on these issues.

After establishing that the pure Heisenberg model lies

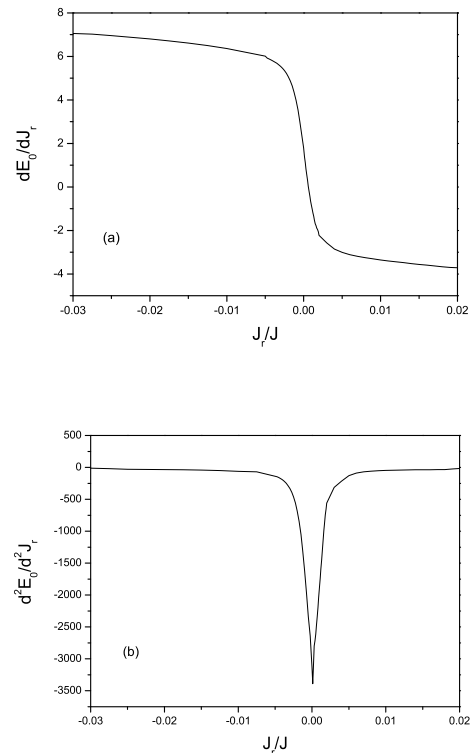


FIG. 3: The first (a) and the second (b) derivative of the ground state energy as a function of  $J_r$ .

at a quantum critical point, we now move to the question what state the ring exchange coupling will drive the system into. For this purpose, we have examined the spin-spin correlation and dimer-dimer correlation function. The comparison of the spin correlation function between the pure Heisenberg model and the model with  $J_r/J = 0.15$  for all the 10 inequivalent distances on the 36-site cluster is tabulated in Table I. The numbering of sites are the same as that used in Ref[7] and we also use site 26 as the reference site. The main difference between the pure Heisenberg model and the  $J_r = 0.15J$  system can be summarized as follows. The spin correlation between spins on the same hexagonal ring (site 14 and site 15) is enhanced by the ring exchange coupling, while those outside the same hexagonal ring is in general reduced. This results in a more short-ranged spin correlation function. This can be seen more clearly in Fig. 5, in which we plot the absolute value of the spin correlation between the reference site 26 and all other sites.

To see if there is any qualitative difference in the spin correlation between the pure Heisenberg model and the model with non-zero ring exchange coupling, we have calculated the spin structure factor at both  $J_r = 0$  and

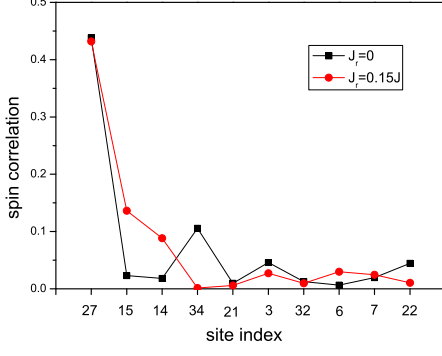


FIG. 4: The absolute value of the spin correlation function between the reference site 26 and all the 10 symmetry inequivalent sites on the 36-site cluster. The ordering of the sites in the figure is determined by their distance with site 26. When such distance is degenerate (for example, site 14 and 34), the site on the same hexagonal ring as site 26 appear earlier in the ordering.

$J_r = 0.15J$ . The spin structure factor is defined as

$$S(q) = \sum_{i,j} e^{iq \cdot (R_i - R_j)} \langle S_i \cdot S_j \rangle. \quad (2)$$

On the finite cluster, care should be paid on the choice of the wave vector  $\vec{q}$ . In the lower panel of Fig.1, we have plotted the translational unit of the 36-site cluster, on which periodic boundary condition is imposed. Under such boundary condition, the allowed momentum can be generally written as

$$\vec{q} = q_x \vec{b}_1 + q_y \vec{b}_2, \quad (3)$$

in which  $\vec{b}_{1,2} = 2\pi(1, \pm \frac{1}{\sqrt{3}})$  denotes the two primitive reciprocal vectors of the triangular lattice from which the Kagome lattice is derived by removing one fourth of lattice sites.  $q_x = \frac{m}{12}, q_y = \frac{n}{12}$  with  $m, n = 0, \dots, 12$ . Although there is clearly redundancy in the momentum mesh Eq.(3) for the description of spatial variation on the 36-site cluster, it presents a natural way to understand the evolution of the spin correlation pattern on the Kagome lattice, as will be clear below.

The spin structure factor for the pure Heisenberg model and the model with  $J_r = 0.15J$  are shown in Fig.6. For the pure Heisenberg model, the spin structure factor peaks at three independent momentum  $(q_x, q_y) = (0, 1/2), (1/2, 0), (1/2, 1/2)$ . This structure is caused by the antiferromagnetic correlation between nearest neighboring spins in the three directions. For the  $J_r = 0.15J$  case, the peak of the spin structure factor moves to  $(q_x, q_y) = (1/3, 1/3)$ , or to the momentum  $\vec{q} = (\frac{4\pi}{3}, 0)$ . This momentum is characteristic of the coplanar local spin correlation on triangular lattice with 120 degree an-

gle between neighboring spins on each triangular plaquette (it is interesting to note that the 36-site cluster studied in this paper can host such a momentum). At the same time, the peak in the spin structure factor is found to be more rounded than the pure Heisenberg model, indicating that the spin correlation is more short ranged, which is completely consistent with the result shown in Fig.5.

TABLE I: The spin correlation function between the reference site 26 and all the 10 symmetry inequivalent sites on the 36-site cluster.

$n$	$r$	$J_r = 0$	$J_r = 0.15J$
27	1	-0.43838	-0.43193
15	$\sqrt{3}$	0.02314	0.13637
14	2	-0.01802	-0.08841
34	2	0.10547	0.00157
21	$\sqrt{7}$	-0.00956	-0.0058
3	3	-0.04597	-0.02732
32	$2\sqrt{3}$	0.01257	-0.00959
6	$2\sqrt{3}$	0.00636	-0.0299
7	$\sqrt{13}$	-0.01967	0.02467
22	4	0.04443	-0.0104

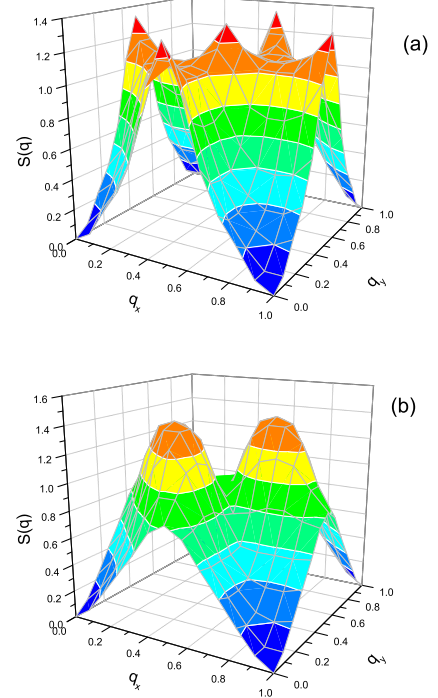


FIG. 5: The spin structure factor for the (a) pure Heisenberg model and (b) the model with  $J_r = 0.15J$ .

Now we turn to the dimer-dimer correlation to see if the ring exchange coupling would drive the system into a state with spin Pereils type order with broken transla-

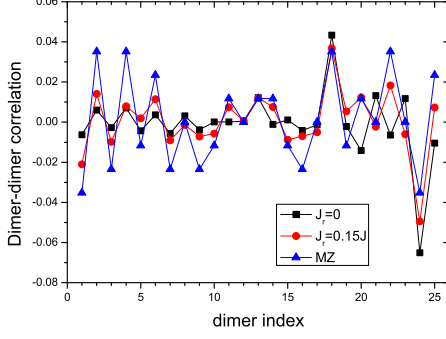


FIG. 6: The dimer-dimer correlation function between the reference dimer on bond (25, 26) and all the 25 inequivalent dimers on the 36-site cluster. The bonds on which these dimers reside are listed in Table II. Here  $(k, l)$  means that the dimer links site  $k$  and site  $l$ . MZ denotes the results of the Marston-Zeng spin Pereils solid state.

tional symmetry, which is hotly debated in the literature. The dimer-dimer correlation function is defined as follows

$$C(i, j; k, l) = \langle (S_i \cdot S_j)(S_k \cdot S_l) \rangle - \langle S_i \cdot S_j \rangle \langle S_k \cdot S_l \rangle. \quad (4)$$

As in Ref[7], we choose the bond between site 25 and 26 as the reference dimer and calculated the correlation between all the 25 inequivalent dimers with this reference dimer. The results is tabulated in Table II. As first noticed in Ref[7], the dimer correlation in the pure Heisenberg model modulates at large distance in close resemblance with a special kind of spin Pereils solid state(the Marston-Zeng(MZ) spin Pereils solid state)[21], although the amplitude of the modulation is much weaker. In the MZ spin Pereils solid state, as energy can be reduced by dimer resonance, the system prefers dimer coverings with the maximal number of 'perfect hexagon's, on each of which two dimer configurations(both with three dimers on the hexagon) can resonant between each other. On the 36-site cluster studied in this paper, there can be at most two 'perfect hexagon's. As such a state has a smallest unit cell containing 36 sites, Fourier transform on the dimer-dimer correlation function on our cluster can not help to understand such a ordering tendency. We thus compare directly the modulation pattern in the real space. In Figure 7, we compare the dimer-dimer correlation of the pure Heisenberg model and the model with  $J_r = 0.15J$  with the result of the MZ spin Pereils solid state. As can be seen clearly from the figure, the resemblance between the modulation pattern with the MZ solid state is greatly enhanced by the ring exchange coupling. This is in fact not at all unexpected, as the the ring exchange coupling also encourages resonance processes around the hexagons. However, as MZ ordering pattern has a primitive unit cell with 36 sites, our result on the 36-site cluster can not say anything about the long

TABLE II: The dimer-dimer correlation function between the reference dimer on bond (25, 26) and all the 25 inequivalent dimers on the 36-site cluster. MZ denotes the results of the Marston-Zeng spin Pereils solid state.

$n$	$(k, l)$	$J_r = 0$	$J_r = 0.15J$	MZ
1	(5, 6)	-0.00628	-0.02105	-0.03516
2	(4, 5)	0.00603	0.01403	0.03516
3	(3, 4)	-0.00273	-0.0098	-0.02344
4	(3, 8)	0.0071	0.00793	0.03516
5	(4, 8)	-0.0043	0.00196	-0.01172
6	(5, 9)	0.00366	0.0114	0.02344
7	(9, 14)	-0.00559	-0.00909	-0.02344
8	(8, 13)	0.00315	-0.00139	0
9	(8, 12)	-0.00384	-0.00718	-0.02344
10	(11, 12)	1.56504E-4	-0.00568	-0.01172
11	(12, 13)	9.65042E-5	0.00744	0.01172
12	(13, 14)	4.56504E-4	4.99119E-4	0
13	(14, 15)	0.01221	0.01209	0.01172
14	(14, 19)	-0.00113	0.00759	0.01172
15	(13, 19)	0.00108	-0.0088	-0.01172
16	(11, 18)	-0.00418	-0.00698	-0.02344
17	(18, 22)	-0.00133	-0.00505	0
18	(19, 24)	0.04337	0.03681	0.03516
19	(22, 23)	-0.00214	0.00532	-0.01172
20	(23, 24)	-0.01415	0.01233	0.01172
21	(23, 29)	0.01322	-0.00225	0
22	(29, 32)	-0.00645	0.01831	0.03516
23	(32, 33)	0.01178	-0.00603	0
24	(34, 35)	-0.06509	-0.04946	-0.03516
25	(1, 33)	-0.01045	0.00731	0.02344

range behavior of such ordering tendency.

The result presented above can be summarized as follows. First, the pure Heisenberg model on Kagome lattice is found to be lying exactly at a quantum critical point and the excitation gap in both spin channel and the singlet channel should vanish in the thermodynamic limit. The ring exchange coupling is found to drive the system into a state with more short ranged spin correlation. Such a spin disordered state has a local spin correlation pattern in close resemblance with the antiferromagnetic Heisenberg model on triangular lattice. At the same time, the state exhibits dimer correlation in close resemblance with the MZ spin Pereils solid state, although the long range ordering can not be decided with our results.

Many issues remains open. In particular, it is interesting to know if MZ spin Pereils modulation pattern enhanced by the ring exchange coupling would solidify into a static order in the thermodynamic limit. This can in principle be answered by methods such as series expansion calculation. If the modulation remains dynamical, then it is quite likely that the ring exchange coupling

has really drive the system into a incompressible quantum liquid state, which is long sought by the researchers in this field. Another issue is about the nature of the criticality of the pure Heisenberg model, especially, it is interesting to know if the anomalous singlet dynamics survive in the thermodynamic limit and how it contribute to the critical behavior. Finally, we note that as the pure Heisenberg model sit at a quantum critical point, it is important to take into account the effect of the ring exchange coupling when compare the experimental result with theory, as the ring exchange coupling on the hexagons stands as the most relevant deviation from the Heisenberg limit. It is interesting to know how the ring exchange coupling will change the low energy dynamics of the system, especially in the singlet channel. Our preliminary full spectrum calculation on 18-site cluster implies that the low energy spectral weight in both the singlet channel and the triplet channel are reduced with increasing strength of ring exchange coupling. However, result from larger cluster and/or from other techniques are obviously needed to settle down this issue.

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